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EVALUATION OF RIVER LOAD ESTIMATION METHODS FOR TOTAL PHOSPHORUS

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ABSTRACT. Accurate estimates of pollutant loadings to the Great Lakes are required for trend detection, model development, and planning. On many major rivers, infrequent sampling of most pollutants makes these estimates difficult. However, most large rivers have complete daily flow records available from the U.S. Geological Survey. A number of different estimation methods have been developed to use these data in conjunction with available concentration data to calculate pollutant loadings. Several of these methods have been evaluated in this paper for a typical major tributary.

Intensive measurements of pollutant loadings to Lake Michigan from the Grand River in 1976-1977 were conducted by USEPA, Region V. Daily concentrations of several chemical parameters, including total phosphorus, were determined. This information, together with daily river flow rates from USGS, provide an excellent data set for testing various load estimation methods. Ten different methods were tested using 680 randomly generated 25-sample subsets of the daily total phosphorus data set. The methods tested included several simple calculation schemes, as well as flow-concentration correlations and the stratified ratio estimator. The latter method is shown to be at least slightly better than the others for these data and for this type of sampling, including when sampling is concentrated during periods of high flow.

INTRODUCTION

On November 22, 1978, the governments of the United States and Canada signed the Great Lakes Water Quality Agreement (IJC 1978). Annex 3 of that agreement, entitled "Control of Phosphorus," specifies in quantitative terms what the future phosphorus load to each Great Lake and major embayment must be to meet the goal of minimizing problems stemming from eutrophication. As phosphorus reduction efforts begin to be implemented in the Great Lakes basin, it is extremely important to monitor progress toward these objectives in as accurate a manner as possible.

Phosphorus mass balance models (Lorenzen *et al.* 1976, Chapra 1977, Chapra and Sonzogni 1979) require the best possible loading information for model calibration and verification. Open lake trends for phosphorus can be detected earlier, and with more accuracy, if reliable loadings are available (DePalma, Canale, and Powers 1979). Therefore, the best possible load estimation method

should be used to develop this information, and this method should be standardized so that there is no difference in its application among jurisdictions.

An obvious way to improve load estimates is to take as many concentration samples as possible from the tributary of interest. Unfortunately, due to the large number of Great Lakes tributaries, this is an expensive and difficult task. Many streams are only sampled twice per month, at best. However, most major streams around the Great Lakes have complete daily flow records available from the U.S. Geological Survey. Previously, the flows for the days on which concentrations were sampled were multiplied by the respective concentrations to calculate daily loading rates. These values were averaged over the year to produce the annual mean loading rate. This method ignores the extra information contained in the data for flow on days when no concentration sample was taken. Since the loading rate of phosphorus is highly dependent on flow, substantial errors could result from using such a method if the sampling occurred during

times of low flow. Therefore, given the constraint of few concentration samples, some load estimation method is needed to make use of all available information and produce estimates of acceptable accuracy.

The purpose of this paper is to consider a Great Lakes tributary that has been intensively sampled and treat it as though only a few samples were available in order to test 10 different load estimation methods. These methods are described and then compared on the basis of three evaluation criteria. The methods judged to be best are tested further and compared.

STUDY SITE: GRAND RIVER

Intensive measurements of pollutant loadings to Lake Michigan from the Grand River were directed by the Surveillance and Analysis Division of USEPA, Region V. Daily concentrations of several chemical parameters, including total phosphorus, were determined. This information, together with daily river discharge rates obtained from the U.S. Geological Survey, Water Resources Division, provides an excellent data set for testing the various load estimation methods.

The Grand River is located in west-central Michigan. Its source is near Jackson, Michigan, and it flows west and north via Lansing and Grand Rapids before it discharges to Lake Michigan at Grand Haven. The sampling station is located at Eastmanville, just west of Grand Rapids. This site is still 20 miles upstream of the mouth, but the drainage area at this point is 13,550 km² (5,230 mi²). The average discharge for the period of record at Grand Rapids was 101 m³/sec (3,580 cfs). The mean discharge for water year 1976, however, was 161 m³/sec (5,690 cfs) (U.S. Geological Survey 1977). The study period for which flow and concentration information coincided was March 1, 1976, to February 28, 1977.

The hydrograph for the study site for this time period is shown in Figure 1. The study site experienced substantially higher than average flows during this period. A plot of total phosphorus concentration vs. flow is shown in Figure 2.

The Grand River basin is dominated by cropland (Great Lakes Basin Commission 1976). As a result, the phosphorus loads to Lake Michigan are fairly high. In 1976, the load, as calculated at the study site, was about 9.4% of the total phosphorus load to the lake.

The total phosphorus loading has been calcu-

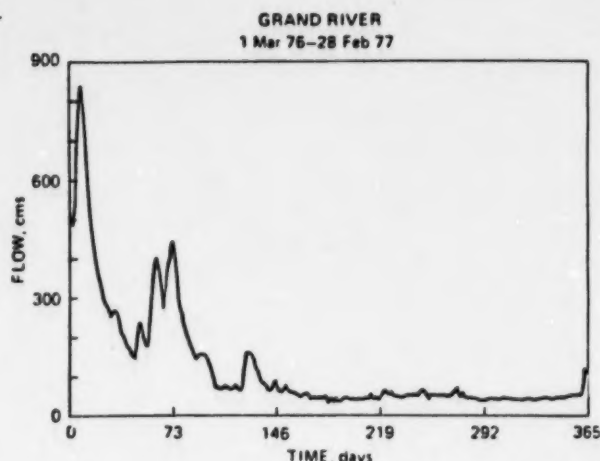


FIG. 1. Grand River hydrograph, 1 Mar/1976 - 28 Feb/1977.

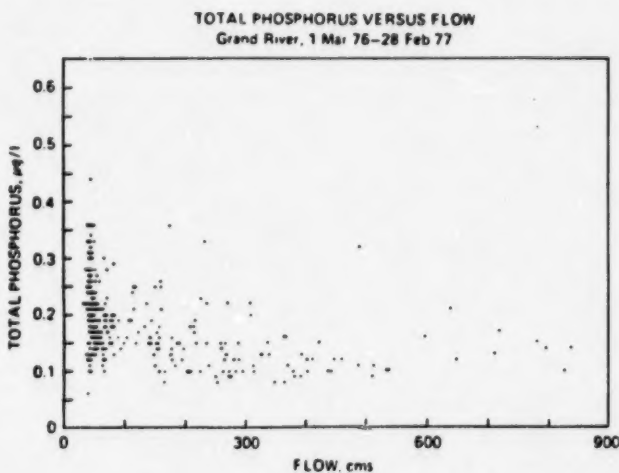


FIG. 2. Scatter plot of total phosphorus concentration vs. flow, Grand River, 1 Mar/1976 - 28 Feb/1977.

lated on a daily basis for the study site (Figure 3). The mean annual load was 1,730 kg/day. The study period was then "sampled" by randomly generating 25 sampling dates to produce subsets of the data set on which the different estimation methods could be tested. The number of sampling dates to be used was arbitrary, but 25 was chosen to roughly correspond to the number that would be obtained with a bi-weekly sampling frequency.

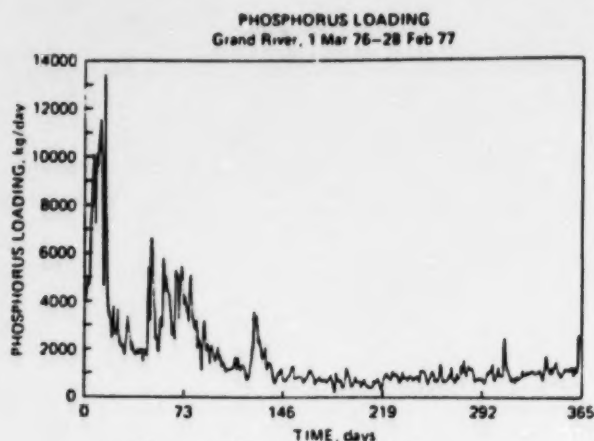


FIG. 3. Total phosphorus loading time series, Grand River, 1 Mar/1976 - 28 Feb/1977.

METHODS

There are many methods of load estimation. This paper will consider only those methods that can be used when the number of concentration samples for a stream is 50 or less and the daily flow record is available. This corresponds to the data base available for many tributaries around the Great Lakes. Most states have tributary monitoring programs with a sampling frequency of once per month or greater and, as mentioned previously, the U.S. Geological Survey maintains stage height gages near the river mouths of most streams of interest. In fact, as part of the study on Great Lakes pollution from land use activities, data of this type were used to estimate mean annual total phosphorus loads for 110 major U.S. Great Lake tributaries (Sonzogni *et al.* 1978).

Three types of methods will be considered. The first and most straightforward involves means of either loads or concentrations over a certain time period, while the second uses simple log-linear regressions to estimate daily concentrations during a certain time period. The third type is the stratified ratio estimator suggested by J. L. Clark (personal communication to C. Timm, IJC, 1977). All methods will be used to calculate mean annual loads. Some of the methods described below are more appropriate than others for estimating loads in shorter time periods, however, only annual means are considered here.

Methods of the first type will be referred to as "simple" and denoted as methods 1 thru 5. These

methods can be described in general by the following equation:

$$L_i = \frac{2.45 \sum_{j=1}^{365} A_j C_{ij} Q_j}{\sum_{j=1}^{365} A_j} \quad (1)$$

Where: L_i = the mean annual load estimate for the i th method

A_j = either one or zero depending on whether a concentration (estimate or actual) is available on that day (1=available, 0=not available)

C_{ij} = the concentration on day j from method i , in mg/L

Q_j = the flow on day j , in cfs

2.45 = a conversion factor to convert from mg/L and cfs to kg/day

The five methods define the concentration as follows:

$$i = 1: \quad C_{ij} = C_j \quad \text{if} \quad A_j = 1 \quad (2)$$

Where: C_j is the actual measured concentration on the j th day.

$$i = 2: \quad C_{ij} = H_k \quad (3)$$

Where:

$$H_k = \frac{\sum_{j=1}^{31} A_j C_j}{\sum_{j=1}^{31} A_j} \quad \text{if} \quad 1 \leq j \leq 31 \quad (4)$$

$$H_k = \frac{\sum_{j=32}^{60} A_j C_j}{\sum_{j=32}^{60} A_j} \quad \text{if} \quad 32 \leq j \leq 60$$

etc. to $j = 365$
(i.e. H_k 's are monthly means)

- i = 3: same as i = 2 except H_k 's are quarterly means
 i = 4: same as i = 2 except H_k 's are semi-annual means
 i = 5: same as i = 2 except H_k is the annual mean

The second type of methods will be referred to as the "complex" methods. These methods use linear regressions of concentration on log flow. The C_{ij} 's in equation (1) are calculated from these regressions as follows:

- i = 7: the regression is performed for all C_j 's in a given quarter
 i = 8: the regression is performed using data for each half of the year
 i = 9: one regression is performed using all data from the whole year
 i = 10: two regressions are performed: one in each "flow stratum" as specified by the user. Flow strata are subsets of the available data set based on the magnitude of the flow.

For methods 7 through 10, the natural logarithm of the daily average flow is substituted into the appropriate regression equation and the resulting concentration estimate is used in the load estimate (equation (1)).

Other regressions of concentration on some function of flow were considered, such as those involving the inverse of flow (Manczak and Florczyk 1971). No regression was found with a higher statistical significance than concentration vs. natural log flow; therefore, only this regression is used in this evaluation.

The use of the ratio estimator for estimating pollutant loadings was suggested by J. L. Clark (personal communication to C. Timm, IJC, 1977). The ratio estimator was developed by Beale (1962) and discussed further by Tin (1965) and Kendall and Stuart (1968). It is defined as follows:

$$\bar{\mu}_y = \mu_x \frac{m_y}{m_x} \left(\frac{1 + \frac{1}{n} \frac{S_{xy}}{m_x m_y}}{1 + \frac{1}{n} \frac{S_x^2}{m_x^2}} \right) \quad (5)$$

where

$\bar{\mu}_y$ = ESTIMATED LOAD

μ_x = mean daily flow for the YEAR

m_y = mean daily loading for the days on which concentrations were determined

m_x = mean daily flow for the days on which concentrations were determined

n = number of days on which concentrations were determined

$$S_{xy} = \frac{1}{(n-1)} \sum_{i=1}^n x_i y_i - n m_x m_y$$

$$S_x^2 = \frac{1}{(n-1)} \sum_{i=1}^n x_i^2 - n m_x^2$$

x_i = individual measured flows

y_i = daily loading for each day on which concentration was determined

The estimate is derived from a ratio, m_y/m_x , which is the ratio of the mean of measured loads to the mean of flows when loads were measured. This ratio is used with the mean of the actual flow, μ_x , to obtain the estimate. Thus, this method is ideally suited to those situations where there is an abundance of flow information for a tributary, but relatively little concentration information.

The ratio estimator is termed unbiased since the mean of several ratio estimates tends toward the "true" mean. The bias in the estimate is removed by the term in brackets in equation (5). Note that as n , the number of days concentration measurements are available, increases, the influence of the bias correction term decreases.

The calculation of the ratio estimator has been stratified as was the linear regression in Method 10. This was also suggested by J. L. Clark (personal communication to C. Timm, IJC, 1977) to further improve the estimate. A discussion of the subject of stratification can be found in Cochran (1977). The application of this type of estimate by strata is shown to reduce the error of the estimate. The choice of the number and size of the strata to be used is a complex subject and requires further research. In this paper the use of strata will be confined to two: high flow and low flow. The division between the two is a matter of judgement.

The above methods have been tested using the criteria described in the next section. Each calculation for an individual method was performed 680 times using sets of 25 randomly determined dates (or sampling days). The results were tabulated and evaluated. Certain subsets of these results were

examined further for methods of each type that were most successful.

EVALUATION CRITERIA

Figure 4 illustrates two useful concepts for establishing criteria for evaluating and comparing the different methods. The bias of a method is defined as the expected value of the estimate minus the true value (Figure 4a). It measures how far and in what direction the center of the observed distribution is from the true value (Bickel and Doksum 1977).

STATISTICAL CONCEPTS FOR EVALUATING LOAD ESTIMATION METHODS

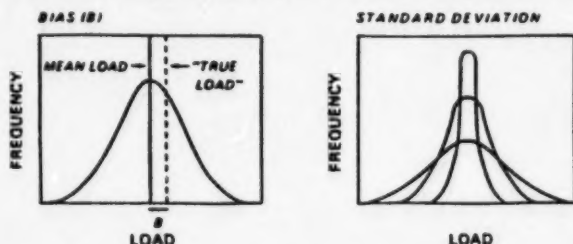


FIG. 4. Statistical concepts for load estimation method evaluation criteria. A. Bias is the difference between the "true" load and the mean of the distribution of the estimates. Standard deviation reflects the precision of the estimate. B. The broader distributions have higher standard deviations.

Non-zero values of bias are an indication of a systematic fault in the method. Methods with high bias should be avoided since the estimate will be in error no matter how many samples are taken.

The standard deviation measures how tightly the distribution of the estimate is clustered about its center. This is sometimes referred to as the estimate's precision. In Figure 4b, the broader distributions have larger standard deviations and low precision. It is obviously desirable to have a load estimate with high precision since the confidence interval for the estimate will be small.

These two statistical concepts can be combined to give one overall criterion: the root mean square error (Bickel and Doksum 1977). This quantity is defined as follows:

$$\text{R.M.S.E.} = \sqrt{B^2 + S^2}$$

Where: B is the bias of the method, and
S is the standard deviation of the method.

The R.M.S.E. is an excellent criterion because it allows tradeoffs between bias and precision. For example, if it is possible to greatly improve the precision for only a slight increase in bias, then the R.M.S.E. will reflect the actual gain. This criterion is therefore used in this paper to evaluate the different types of load estimates.

It should be noted that the true annual average load is considered to be a "known" quantity. Naturally, the actual load can never be known exactly but the data used for the calculation are so extensive compared to the typical load estimation data set that the assumption that this quantity is known has been made. Figure 5 shows the frequency distribution of total phosphorus loads in the time period March 1, 1976, to February 28, 1977. This distribution is badly skewed to the right, a typical situation for large rivers. If the true load were not known, the selection of a minimum variance unbiased estimate of the load on theoretical grounds would not be straightforward since this distribution is obviously not normal.

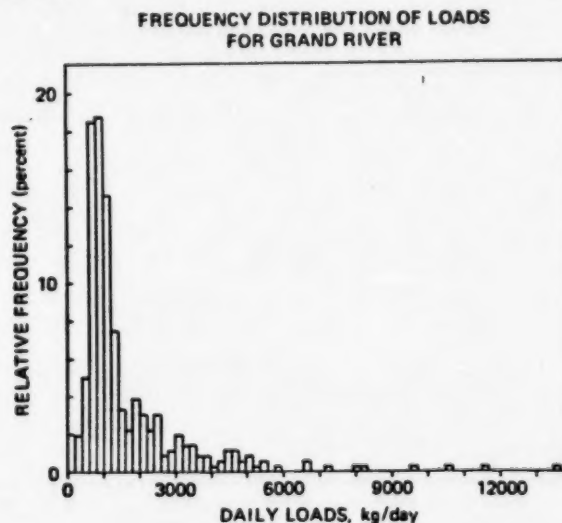


FIG. 5. Frequency distribution of daily total phosphorus loads for Grand River, 1 Mar/1976 - 28 Feb/1977.

RESULTS

Simple Methods

The results of load estimation using the simple methods illustrate the concept of tradeoff between

TABLE 1. Comparison of evaluation criteria for "simple methods." Number of calculations = 680.

Method	Description	Bias (kg/day)	Standard deviation (kg/day)	Root mean square error (kg/day)
1	Daily flow X daily concentration	+12	337	337
2	Daily flow X monthly average concentration	+22	191	192
3	Daily flow X quarterly average concentration	+29	157	159
4	Daily flow X semiannual average concentration	+134	130	186
5	Daily flow X annual average concentration	+346	151	377

TABLE 2. Comparison of evaluation criteria for "complex methods." Number of calculations = 680.

Method	Description	Bias (kg/day)	Standard deviation (kg/day)	Root mean square error (kg/day)
7	Daily flow X conc. from quarterly regression on log flow	-8	206	206
8	Daily flow X conc. from semiannual regression on log flow	-4	164	164
9	Daily flow X conc. from annual regression on log flow	-30	159	162
10	Daily flow X conc. from stratified regression on log flow	-34	178	181
Beale's ratio estimator	Stratified	+0.6	160	160

bias and precision (Table 1). As the time period over which the concentration is averaged increases, the bias increases but the standard deviation generally decreases. The R.M.S.E. combines both concepts and is at a minimum for method 3. The rest of the methods are rejected on this basis, and only method 3 is considered for further evaluation.

Complex Methods (including ratio estimator)

All of the complex methods of estimation perform reasonably well (Table 2). The ratio estimator is best for all three criteria. Methods 8 and 9 are also quite adequate. The ratio estimator and method 8 are chosen for further evaluation. Method 9 could also have been selected, but method 8 is expected to be more responsive to the effects considered in the next section.

Further Evaluation

One of the problems of river load estimation that all of these methods are designed to correct (except method 1) is the possibility that the results have been unduly affected by flow. A preponderance of either high-flow samples or low-flow samples could

lead to inaccurate estimates. For the case of the present study, the mean river flow was 127 m³/sec (4,480 cfs) and the median flow was 56.5 m³/sec (2,000 cfs). The cutoff between high and low flow was set at 113 m³/sec (4,000 cfs). There were 254 days, then, that were considered to have low flow (i.e. 69.6% of the year). If, by chance, only 3 days of the 25 sampled were high-flow days, then 88% of the data used in the estimate would be from low-flow days. If the method to be used does not take this problem into account, the estimate may be very inaccurate. Therefore, the three remaining methods were further evaluated to see how they performed with this type of difficulty.

The problem was simulated by selecting only those estimates that had a large number of either high- or low-flow days in the 25-day sample. The cutoff for "low-flow samples" was 19 low-flow days or more, while that for "high-flow samples" was 9 high-flow days or more. This resulted in 242 high-flow calculations and 222 low-flow ones. The three criteria were recalculated for each flow condition (Table 3). On the basis of R.M.S.E., the ratio estimator is slightly better for both conditions. There is a small bias for this method, but it is more than compensated for by the higher precision.

TABLE 3. Comparison of evaluation criteria for methods 3 and 8 and the ratio estimator under the assumptions of high- and low-flow sampling.

Method	High-flow samples (9 or more) Number of Calculations = 242			Low-flow samples (19 or more) Number of Calculations = 222		
	Bias (kg/day)	Standard deviation (kg/day)	Root mean square error (kg/day)	Bias (kg/day)	Standard deviation (kg/day)	Root mean square error (kg/day)
3	+30	138	142	+28	174	176
8	+0.5	144	144	-10	180	180
Ratio estimator	+5	141	141	-8	172	172

DISCUSSION

The previous simulation of high- and low-flow sampling days demonstrates the desirability of obtaining as many high-flow samples as possible when any of the three methods are used. The precision of the estimates improves substantially as the number of days of high flow in the data set increases (Tables 1-3). This could be put into practice by identifying probable high- and low-flow months for a particular stream and then intensifying the sampling effort in the high flow months, i.e. stratified sampling.

It should be noted that all of the methods considered except 1, 5, and 9 use stratification of the samples to improve the estimate. Methods 2, 3, 4, 7, and 8 are stratified by time and method 10 and the ratio estimator are flow stratified. Actually, stratification with time is simply a crude way of obtaining flow stratification. The poor performance of some of these methods is due, in part, to inadequate stratification.

Examination of Tables 1-3 reveals that the ratio estimator is not the clear choice for the best method for load estimation calculations for this data set. This is partly due to the "stable" nature of the Grand River hydrology. Much of the wild variation that this method was designed to correct does not occur in the Grand River, at least in the period under study. In addition, as the number of methods used in a study such as this increases, the chances of finding a method that works well on a particular data set also increases. Experience (Bierman *et al.* 1980) with several parameters and many years of data for the Saginaw River (in Michigan) has shown that methods 7-10 lead to poor estimates and that method 2 is almost always superior to method 3. However, the ratio estimator consistently gave the best results.

The ratio estimator used in this analysis was designed to be unbiased. It was the only method that remained substantially unbiased after 680 calculations. It is possible that some of the other methods could be corrected for bias; however such a correction is not straightforward.

Another criterion for evaluation of these estimation methods is the observed population's skewness. This is a measure of the asymmetry of the distribution. All of the methods give populations of estimates that are positively (right) skewed. However, the skewness of the ratio estimator is the least of all methods except for methods 4 and 5 which are excessively biased.

CONCLUSIONS AND RECOMMENDATIONS

On the basis of the root mean square error, the unbiased stratified ratio estimator has been shown to be better than most of the methods considered in this study for this set of data. It is recommended that this method be used to estimate tributary loads for total phosphorus when concentration data are limited and the daily flow record is available.

If the concentration data for a tributary are the result of bi-weekly sampling throughout the year, the situation is likely to correspond to the low-flow sampling case in Table 3 (i.e. 19 or more low-flow samples). In this case, the ratio estimator will give the best estimate for the annual average load. If the tributary is then subjected to stratified sampling, Table 3 indicates that, while all three methods improve substantially for the high-flow case, the ratio estimator still gives a slightly better estimate.

The utility of this method for parameters other than phosphorus has not been checked. In general,

however, any flow-sensitive parameter that is significantly affected by stream flow rate should be estimable by this method. This evaluation is directly applicable only to the Grand River. It is expected that other streams with similar characteristics would also be amenable to this type of estimation. This kind of estimation would probably not be appropriate for excessively variable streams in which daily flows vary by a factor of 100 or more.

As the number of concentration samples taken increases, the results of the estimation methods considered in this study will all converge to the actual annual mean load. As the number of concentration samples decreases, however, disagreement between the estimates should be greater. In fact, some methods need a certain minimum number of samples to even be able to calculate an estimate. As long as there exists an estimate of the load in each stratum, the stratified ratio estimator should give reasonable estimates.

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